Modeling of Cascades and Sub-cascade Formation in Materials Irradiated by Fast Charged Particles on Accelerators and by Fast Neutrons Using Fission and Fusion Energy Spectra

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Abstract. A new theoretical model is developed and used for the investigation of cascades and sub-cascade formation in fission and fusion structural materials under fast neutron energy spectra corresponding to the fission and fusion reactors and fast charged particle irradiations. The developed model is based on the analytical consideration of elastic collisions between displaced moving atoms and target atoms into atomic cascades produced by a primary knock-on atom (PKA) with the some kinetic energy getting from fast charged particles and fast neutron irradiations. The criterion of sub-cascade formation is based on the comparison of two calculated values: mean distance between two consequent PKA collisions and the size of sub-cascade produced by PKA.The Tomas-Fermy interaction potential is used for the describing of elastic collisions between moving atoms and target atoms. The suggested model takes into account electronic losses of moving atoms between elastic collisions during the scattering process. The analytical relations for the most important characteristics of sub-cascade are determined including the average number of sub-cascades per one PKA in the dependence on PKA energy. The developed model allows determining the size distribution function of sub-cascades in the dependence on PKA energy. Based on the developed model the numerical calculations for main characteristics of sub-cascades in different materials are performed using the neutron fluxes and PKA energy spectra for fusion reactors: ITER, DEMO and IFMIF-Source. So the total numbers of sub-cascades, distribution functions of sub-cascades in dependence on their sizes and generation rate of sub-cascades for different fission and fusion structural materials: Fe, V, W, Be and C are calculated for these fission and fusion irradiation conditions. The obtained numerical results for main characteristics of cascades and sub-cascade formation under fission and fusion irradiation conditions in these materials are compared with the same results obtained in these materials using different types of fast charged particle irradiations on cyclotron of RRC "Kurchatov Institute".

1. Introduction

In the present paper we develop a self-consistent model to study sub-cascades formation in irradiated materials. This model is partially based on the results of papers [1, 2] and model [3]. This developed model allows calculating the main characteristics of sub-cascades: threshold energy for sub-cascade formation, generation rate of sub-cascades for a given neutron spectrum, average number of sub-cascades per primary knock-on atom (PKA), average distance between sub-cascades, average sub-cascade size. Important efforts have already been carried out to determine the threshold energy E_{sf} for sub-cascade formation. [4] These results are very important for the kinetic consideration of radiation damage (point defects and defect clusters: dislocation loops, voids) accumulation in irradiated materials. Small clusters of radiation defects can form into cascades and sub-cascades after relaxation of them during very short time (10-100 ps) [5]. For the further investigations of an evolution of radiation defect structure in the dependence on an irradiation dose we have to know the generation rate of defect clusters into cascades and sub-cascades for a given fission and fusion neutron spectra. All these values can be obtained using the developed theoretical model in this paper.

The main idea of developed theoretical model is based on the comparison of the mean free path $\lambda(E)$ between two successive collisions of a PKA having a kinetic energy E with the average damage zone size R (an average penetration depth) produced by secondary knock-on atoms (SKA) resulting from the two elastic collisions [3]. The sub-cascades are formed when the following relation is realized $\lambda(E) > R$.

2. Developed model for sub-cascade formation and numerical calculations.

To calculate threshold energy E_{sf} most of the previous approaches [3,6] used the differential cross-section for elastic collisions which characterizes the probability for a moving atom with the energy *E* to get an energy *E'* after an elastic collision. We have to take into account in this model that the secondary knock-on atom (SKA) can get sometimes a kinetic energy *T* higher than the residual energy *E'* of the PKA (and then produces most of the subsequent damage). Thus these approaches are required to determine the energy distribution function for all moving atoms. The present theoretical model for sub-cascade formation is developed for monatomic materials on the basis of our previous paper [3]. This model can also be applied for the consideration of sub-cascade formation in multi-atomic irradiated materials using the system of Boltzmann kinetic equations. [7]

Let us consider the elastic collision between an incident atom with the kinetic energy *E* and a target atom. We suppose here that *E* is higher than the displacement threshold energy ε_d for target atoms $(E>>\varepsilon_d)$. After each collision, the incident atom may have the energy higher or lower than the displaced atom. Because both atoms are undistinguished, we will call the incident atom before collision and the atom with the highest energy after elastic collision as the PKA. In the same way, we will call the atom with the lowest energy after the collision as the SKA. These definitions will allow following the fate of the atom with the highest energy for the subsequent atomic collisions. Provided that *E'* is the highest energy of as-defined PKA after the collision, the two possible configurations are given in *FIG. 1.*

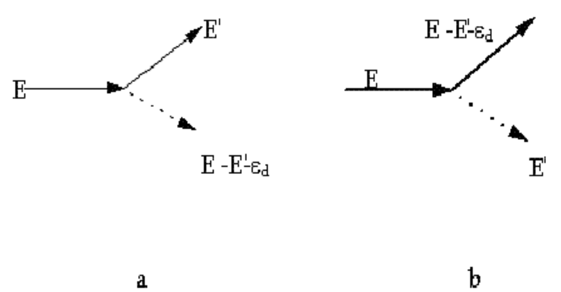

FIG. 1. A scheme of an elastic collision according to our definition of PKA and SKA: a) after collision the incident atom remains as the PKA and has an energy E'; b) after collision the target atom becomes the PKA with an energy E' and the incident atom becomes the SKA.

The elastic cross-section for defined PKA characterizing the type of atomic collisions with the energy transfer higher than certain threshold energy can be easily obtained by using Thomas-Fermi interatomic potential for elastic cross section (see [8]). On the basis of the elastic cross section for defined PKA the mean free path is calculated. On the other hand, the mean damage zone size can be derived from the penetration depth of SKA by averaging over SKA spectrum normalized to unity. Calculations of the penetration depth of SKA take into account inelastic (electronic losses) stopping power determined from the interpolation scheme of electronic energy loss per each atom from high to low SKA energies as proposed by Biersack [9].

The numerical calculations show that there is always a value $E_{sf}=E_{sf}(E)$ for which corresponding damage regions are distinct ($\lambda(E)>R(E,E')$) and the SKA energies in two successive collisions are higher than $E_{sf}(E)$. Thus the formation of sub-cascades in elastic collisions is realized.

A set of numerical calculations have been performed to determine the sub-cascade formation energies and the number of sub-cascades $N_{sub}(E)$ induced by a PKA with the initial energy E in the following fusion structural materials: Fe, Cu, V, C, Al, Be and W. The obtained results for $N_{sub}(E)$ are plotted in *FIG. 2*. It should be remarked that obtained numerical results for the energy dependence of $N_{sub}(E)$ in Cu and Fe (Ni) have a good qualitative and quantitative (20-25%) comparison with the experimental data obtained by M. Kiritani [3] and the Monte-Carlo modeling results of sub-cascade formations for Cu obtained by Heinisch and Sato [1, 2].

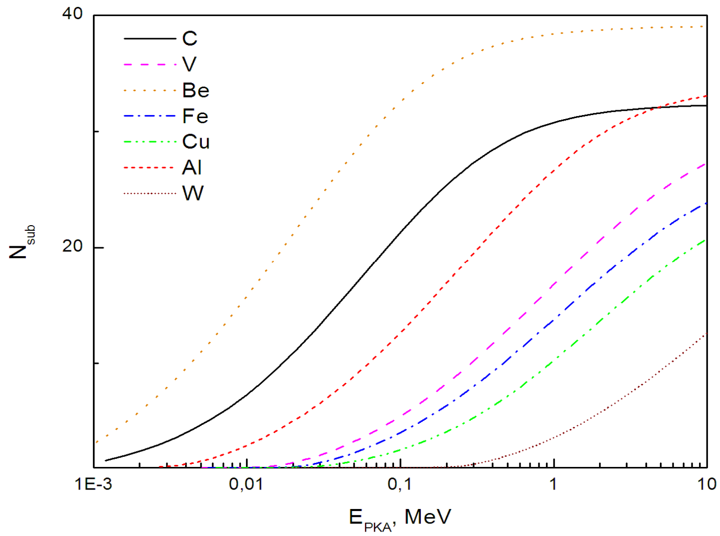

FIG. 2. Number of sub-cascades (N_{sub}) induced by the PKA in Fe, Cu, V, C, Al, Be and W versus PKA initial kinetic energy.

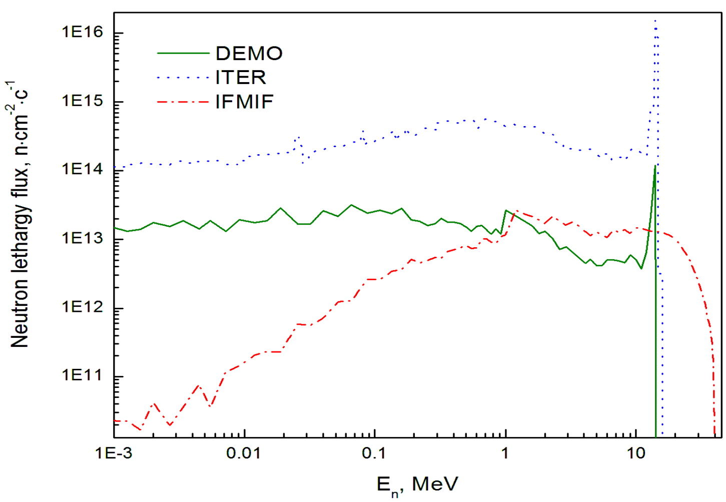

FIG. 3. Neutron spectra for fusion reactors ITER, DEMO and IFMIF -Source

One of the more important characteristic for the sub-cascade formation is their generation rate: the number of sub-cascades produced per unit time and volume for a given neutron spectrum. This determination requires the knowledge of the cross-section for sub-cascades formation Σ_{sf}. Required cross-section was calculated on the basis of elastic neutron scattering using ENDF-VII/B database for Fe, V, C, Be and W materials. The generation rate of sub-cascades has been determined in the listed materials for several neutron spectra (*FIG. 3*) by the integrating of sub-cascade formation cross-section over given spectrum. These two spectra correspond to neutron energy spectra for fusion reactors ITER, DEMO and IFMIF-Source. The calculations have been performed by taking into account both elastic and inelastic (electronic) interactions for PKAs and SKAs. The results for ITER, DEMO and IFMIF spectra are given in *FIG. 4*, *FIG. 5* and *FIG. 6* respectively. The obtained numerical results show that the generation rates of sub-cascade formation for heavy metallic materials: Fe, V and W for ITER fusion spectrum on the order of value is higher comparing with DEMO and two orders higher comparing with IFMIF. These results correlate with the difference of neutron energy spectra (see *FIG.3*). For light materials: C, Be at high neutron energies (higher than 10 keV) this difference has also the one order of value and at low neutron energies (less than 1 keV) this difference stronger (two-three orders of values).

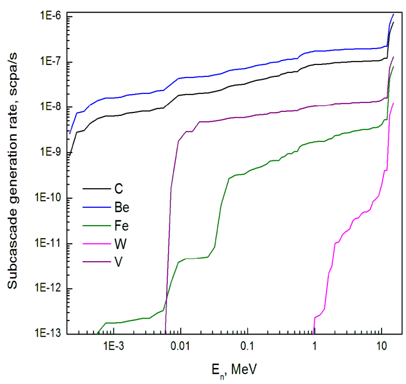

FIG. 4. . Generation rates of sub-cascades versus neutron energy spectrum for ITER.

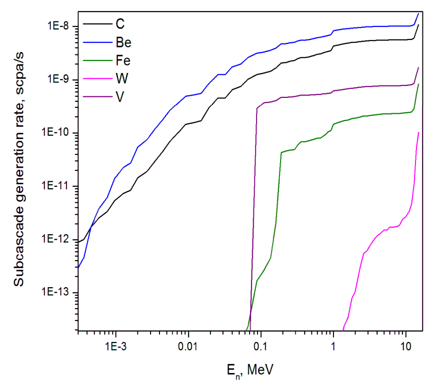

FIG. 5. Generation rates of sub-cascades versus neutron energy spectrum for DEMO.

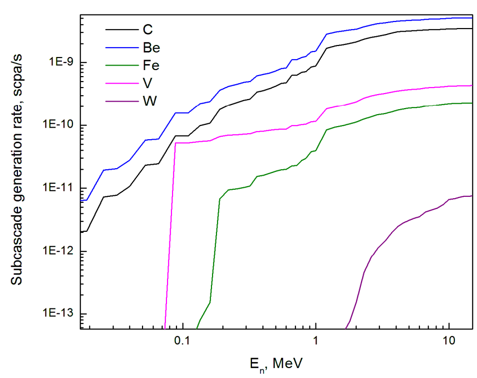

FIG. 6. Generation rates of sub-cascades versus neutron energy spectrum for IFMIF.

The calculations have been made also to determine the generation rates of sub-cascades under fast ion irradiations for carbon and tungsten materials. To determine generation rate the Rutherford cross section was used for ion interactions. Values of 10^{8} ions/cm^2·c was used as fluxes of carbon ions and α-particles. The results of numerical calculations for carbon and tungsten materials are given in *FIG. 7* and *FIG. 8* respectively.

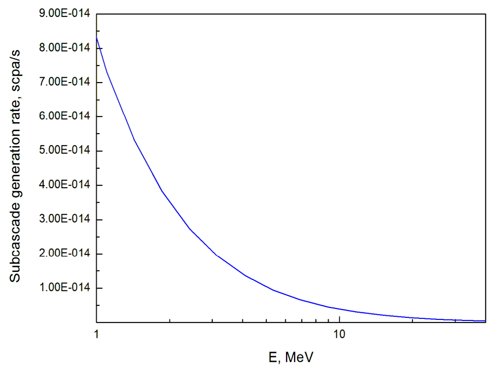

FIG. 7. Generation rates of sub-cascades versus ion energy for graphite irradiated with carbon ions (10^8 ions/cm^2·c)

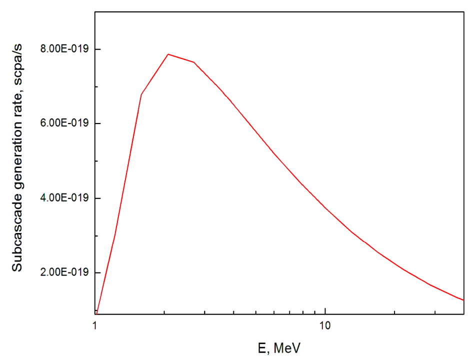

FIG. 8. Generation rates of sub-cascades versus ion energy for tungsten irradiated with α-particles ions (10^8 ions/cm^2·c)

3. Conclusion

Developed model allows to determine the main characteristics of sub-cascades, such as threshold energy for sub-cascades formation, generation rate of sub-cascades for a given neutron spectrum, average number of sub-cascades per PKA, average distance between sub-cascades, average sub-cascade size. Some of these characteristics were also investigated in different fusion structural materials (Fe, C, Be W, V) using the neutron fluxes for fusion reactors ITER, DEMO and IFMIF-Source. The obtained results for PKA energy dependence of number of sub-cascades correlate with the existed experimental data [4] and the numerical Monte-Carlo modeling results of sub-cascade formation in Cu [1, 2]. Results obtained here show that the binary collision model allows to investigating the sub-cascade formation on the collision stage of cascade and give the reasonable results for main important characteristics of sub-cascades as a function of PKA energy. A set of numerical calculations have been made to determine the generation rates of cascades and sub-cascades under fast ion irradiation for carbon and tungsten materials.

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